

4-Hexylresorcinol
136-77-6 | DTXSID1020699

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.66

Global applicability domain: Inside

Local applicability domain index: 5.48e-01

Confidence level: 7.61e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-Hexylresorcinol</div> <div>Measured: 3.45</div> <div>Predicted: 3.66</div>	<div>Image not found</div> <div>2-tert-Butylphenol</div> <div>Measured: 3.31</div> <div>Predicted: 3.34</div>	<div>Image not found</div> <div>6-Chlorothymol</div> <div>Measured: 3.92</div> <div>Predicted: 3.48</div>
<div>Image not found</div> <div>Ibuprofen</div> <div>Measured: 3.97</div> <div>Predicted: 3.66</div>	<div>Image not found</div> <div>Propofol</div> <div>Measured: 3.79</div> <div>Predicted: 4.04</div>	